ALCF EARLY SCIENCE PROGRAM
Mira ESP, Theta ESP gave us
- Breakthrough science
- Technical reports on code porting & tuning
- Open community workshops (science & technology)
- Synergy with Tools & Libraries project
- Stable production platform (problems shaken out)
- Persisting culture of apps readiness for next generation
- Success stories for postdocs
ALCF EARLY SCIENCE PROGRAM (ESP)

Applications Readiness

- Prepare applications for next-gen system:
  - Architecture
  - Scale
- ~Two year lead time

Proposals

- Ambitious targeted science calculation
- Parallel performance
- Development needed
- Team

Support

PEOPLE

- Funded ALCF postdoc
- Catalyst staff member support
- Vendor experts

TRAINING

- Training on HW and programming
- Community workshop to share lessons learned

COMPUTE RESOURCES

- Current ALCF systems
- Early next-gen hardware & simulators
- 3 months dedicated Early Science access
  - Pre-production (post-acceptance)
  - Large time allocation
  - Continued access for rest of year

http://esp.alcf.anl.gov
ESP APPLICATION EFFORTS

Balance of optimization, scaling, development

Next-Generation Cosmology Simulations with HACC: Challenges from Baryons

Code: HACC
PI: Katrin Heitmann (ANL)
N-body gravity + SPH hydro
Catalysts: H. Finkel, A. Pope
Postdoc: J.D. Emberson

- Tune kernel
- Develop CRK-SPY hydro
- Develop subgrid models

First-Principles Simulations of Functional Materials for Energy Conversion

Codes: WEST & Qbox
PI: Giulia Galli (U. Chicago)
MBPT & ab initio MD
Catalyst: C. Knight
Postdoc: H. Zheng

- Use the right optimized libraries
- Address scaling
  - Optimize communication
  - Add 3rd parallelism layer to WEST

Free Energy Landscapes of Membrane Transport Proteins

Code: NAMD
PI: Benoit Roux (U. Chicago, ANL)
MD with replica methods
Catalyst: W. Jiang
Postdoc: B. Radak

- Tune Charm++
- Develop constant-pH
- Develop statistical models

The Hadronic Contribution to the Anomalous Magnetic Moment of the Muon

Codes: MILC & CPS
PI: Paul Mackenzie (FNAL)
Lattice QCD
Catalyst: James Osborn

- Developed/tuned KNL code
- Studied communication issues
FIRST-PRINCIPLES SIMULATIONS OF FUNCTIONAL MATERIALS FOR ENERGY CONVERSION

**Science Impact**
- Properties of materials to be used for solar and thermal energy conversion will be optimized at an unprecedented level of accuracy—by combining ab initio molecular dynamics and post-density functional theory methods—thus providing truly predictive tools, ultimately for device performance, within a MGI material design framework.

**Numerical Methods/Algorithms**
- WEST implements Many Body Perturbation Theory at the GW level, starting from DFT inputs obtained either using GGA or hybrid functionals.
- Qbox is an ab initio molecular dynamics code. It is based on DFT and a plane wave basis.

**Application Development**
- Qbox: optimize FFT (MKL library), evaluate running entirely in MCDRAM
- WEST: vectorization, optimized linear algebra kernels such as DGEMM from MKL

**Case Study: Theta ESP application optimization**

This project will focus on high-performance calculations of nanoparticles and aqueous systems for energy applications. Nicholas Brawand, Institute for Molecular Engineering, University of Chicago
**QBOX OPTIMIZATION**

**SINGLE NODE**
- Strong dependence on libraries
  - Linear algebra
  - FFT
- Replace ScaLAPACK eigenvalue solver with ELPA
  - **5-10X** speedup
- Intel MKL for FFT
- After these optimizations, focus on scaling/multimode issues

**PROCESSOR REMAPPING**
- Different optimal processor maps for linear algebra, FFTs
  - Swap between two layouts
  - Implement custom “gather & scatter” remap
    - 1000X faster than **pgemr2d**

---

Zheng et al., IXPUG Fall 2017, APS March Meeting 2017
**WEST OPTIMIZATION**

**NEW PARALLELISM LAYER**
- Across bands $N_b$ (in addition to across perturbations & plane waves $N_v \times N_z$)
- Good prognosis for 2-5K electron systems on pre-exascale/exascale

**TASK-GROUPS FOR FFTS**
- Distribute independent FFT operations on a smaller number of cores
  - Partition band group into task groups; each fits on single node
  - Shared memory MPI for transpose

---

Zheng et al., IXPUG Fall 2017, APS March Meeting 2017
EXTREME SCALE UNSTRUCTURED ADAPTIVE CFD: AERODYNAMIC FLOW CONTROL

Code: PHASTA • PI: Kenneth Jansen (U. Colorado Boulder) • CFD, unstructured mesh • Catalyst: Hal Finkel

Active synthetic jet actuator

- 3D finite element
- unstructured adaptive mesh
- fully implicit
- 5 billion elements
- 2048 Theta nodes (128K KNL cores)
EXTREME SCALE UNSTRUCTURED ADAPTIVE CFD: AERODYNAMIC FLOW CONTROL

**Code:** PHASTA • **PI:** Kenneth Jansen (U. Colorado Boulder) • CFD, unstructured mesh • **Catalyst:** Hal Finkel
AURORA
Intel Aurora supercomputer planned for 2018 shifted to 2021
Scaled up from 180 PF to over 1000 PF

Support for three “pillars”

Simulation

Data

Learning

Pre-planning review
NRE contract award
Design review
Rebaseline review
Build contract modification

ALCF-3 Facility and Site Prep, Commissioning
ALCF-3 ESP: Application Readiness
NRE: HW and SW engineering and productization
Build/Delivery
Acceptance

AURORA
Hardware and software optimized for Simulation, Data, and Learning

**COMPUTE**
- FLOPS
- Concurrency
- Memory performance
- ML/DL operations

**I/O**
- Speed
- Capacity
- Flexibility
  - Conventional I/O
  - Database
  - Analytics middleware

**Programming Environment**
- Optimizing compilers
- Latest OpenMP
- Key Big Data stack components
- Productivity languages
- ML/DL frameworks
- Optimized libraries
  - Math
  - Statistics
  - ML/NN
**AURORA SYSTEM**

- Nodes will have both high single thread core performance and the ability to get exceptional performance when there is concurrency of modest scale in the code.

- Architecture optimized to support codes with sections of fine grain concurrency (~100 lines of code in a FOR loop e.g.) separated by serial sections:
  - Degree of fine grain concurrency (e.g. number of loop iterations) that will be needed to fully exploit the performance opportunities is moderate. (~1000 for most applications)
  - Independence of these loops is ideal but not required for correctness
  - No limit on the number of such loops; overhead of starting/ending loops is very low

- Serial code (within an MPI rank) will execute very efficiently.

- OpenMP 5 will likely contain the constructs necessary to guide the compiler to get optimal performance.

- The compute performance of the nodes will raise in a manner similar to the memory bandwidth.

- The memory capacity will not grow as fast as the compute:
  - The memory will all be high performance alleviating some concerns of explicitly managing multievel memory & data movement
  - The memory in a node will be coherent

- All compute will be first class citizens: equal access to all resources, memory and fabric etc.

- The fabric BW will be increasing similar to the compute performance for local communication patterns:
  - Global communication BW will likely to not increase as fast as compute performance.
AURORA EARLY SCIENCE PROGRAM
# AURORA ESP SIMULATION PROJECTS

<table>
<thead>
<tr>
<th>Project</th>
<th>PI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Extending Moore’s Law computing with Quantum Monte Carlo</td>
<td>Anouar Benali</td>
</tr>
<tr>
<td>Design and evaluation of high-efficiency boilers for energy production using a hierarchical V/UQ approach</td>
<td>Martin Berzins</td>
</tr>
<tr>
<td>High fidelity simulation of fusion reactor boundary plasmas</td>
<td>C.S. Chang</td>
</tr>
<tr>
<td>NWChemEx: Tackling Chemical, Materials &amp; Biochemical Challenges in the Exascale Era</td>
<td>Thomas Dunning</td>
</tr>
<tr>
<td>Extreme-Scale Cosmological Hydrodynamics</td>
<td>Katrin Heitmann</td>
</tr>
<tr>
<td>Extreme Scale Unstructured Adaptive CFD: From Multiphase Flow to Aerodynamic Flow Control</td>
<td>Kenneth Jansen</td>
</tr>
<tr>
<td>Benchmark Simulations of Shock-Variable Density Turbulence and Shock-Boundary Layer Interactions with Applications to Engineering Modeling</td>
<td>Sanjiva Lele</td>
</tr>
<tr>
<td>Lattice Quantum Chromodynamics Calculations for Particle and Nuclear Physics</td>
<td>Paul Mackenzie</td>
</tr>
<tr>
<td>Metascalable Layered Materials Genome</td>
<td>Aiichiro Nakano</td>
</tr>
<tr>
<td>Free Energy Landscapes of Membrane Transport Proteins</td>
<td>Benoit Roux</td>
</tr>
</tbody>
</table>
## CALL FOR PROPOSALS: A21 ESP DATA, LEARNING PROJECTS

**CFP January 2018**
- Deadline 8 April 2018

**Selections June 2018**
- 5 Data projects
- 5 Learning projects

**Two-year funded ALCF postdoc**

**Cross-cutting proposals** targeting the convergence of simulation, data and learning are very much encouraged.

### DATA
- Experimental/observational data
  - Image analysis
  - Multidimensional structure discovery
- Complex and interactive workflows
- On-demand HPC
- Persistent data techniques
  - Object store
  - Databases
- Streaming/real-time data
- Uncertainty quantification
- Statistical methods
- Graph analytics

### LEARNING
- Deep learning
- Machine learning steering simulations
  - Parameter scans
  - Materials design
  - Observational signatures
- Data-driven models and refinement for science using ML/DL
- Hyperparameter optimization
- Pattern recognition
- Reduced model derivation
- Bridging gaps in theory

---

THANK YOU

Upcoming Program Deadlines

**Aurora Early Science Program for Learning and Data**
Call for Proposals in January 2018

**ADSP Program**
Call for Proposals in April 2018